Int J Life Cycle Assess (2011) 16:803–818
DOI 10.1007/s11367-011-0318-2

LCIA OF IMPACTS ON HUMAN HEALTH AND ECOSYSTEMS (USEtox)

Ecotoxicity impact assessment of laundry products: a comparison of USEtox and critical dilution volume approaches

Gert Van Hoof · Diederik Schowanek · Helen Franceschini · Ivan Muñoz

Received: 7 January 2011 / Accepted: 31 May 2011 / Published online: 13 July 2011

Abstract
Purpose There is an increasing interest in the assessment and comparison of the environmental impacts of consumer products. Schemes such as Grenelle de l'Environnement, currently under development in France, aim to assess and communicate the life cycle impacts of consumer products. Freshwater ecotoxicity is one of the impact categories under consideration. This paper presents the results of a comparison of USEtox and critical dilution volume (CDV) approaches for assessing laundry products.
Materials and methods The study focused only on the end-of-life stage, i.e. when the products are discharged after use into a sewage treatment plant and the environment. Two independent case studies were performed, in parallel, on three laundry product formats: powder, dilute liquid and concentrated liquid. For the USEtox assessment, new characterization factors (ChF) were calculated for all ingredients.
Results and discussion The relative ranking of the laundry product formats was consistent across the two studies but not with the two methods. The dilute liquid format had the highest ecotoxicological impact potential with the CDV method, whereas the powder format was ranked highest with the USEtox method. A comparison was also made between published USEtox factors and those used in this work, suggesting that the published ones should be seen primarily as screening level values.
Conclusions While risk assessment is the recommended method for evaluating the safety of chemicals, the potential use of the CDV and USEtox methods for ranking products on their environmental ecotoxicity profile was evaluated. The two methods showed a lack of agreement, which can be attributed to their different conceptual approaches. The lack of concurrence between the methods raises the issue of whether either method is suitable for environmental product labelling. In addition, the current USEtox database does not cover many laundry ingredients, and furthermore, the USEtox method does not satisfactorily address inorganic chemicals, which are important ingredients in laundry products. The calculation of additional or revised ChFs for USEtox is a time-consuming task. In comparison, the CDV method covers most laundry ingredients, but its lack of comprehensive environmental fate modelling is an inherent weakness. A common limitation for both methods is the level of uncertainty in the impact scores, which can make it difficult to identify statistically significant differences between product scores.

Keywords Critical dilution volume · Ecotoxicity · Environmental product labelling · Laundry detergents · USEtox

Abbreviations

AISE	The European Soap and Detergent Association
C12 AE3S	Alkyl (C12) ethoxysulphate

Responsible editor: Berlan Rodríguez-Perez

Electronic supplementary material The online version of this article (doi:10.1007/s11367-011-0318-2) contains supplementary material, which is available to authorized users.

G. Van Hoof · D. Schowanek
Procter & Gamble, Environmental Stewardship Organisation, BIC,
Temselaan 100,
1853 Strombeek-Bever, Belgium

H. Franceschini · I. Muñoz (✉)
Safety and Environmental Assurance Centre, Unilever,
Sharnbrook MK44 1LQ, UK
e-mail: ivan.munoz@unilever.com

	(3 ethoxy groups)
C14AE7	Alkyl (C14) ethoxylate (7 ethoxy groups)
C25AE3S	Alkyl (C12-C15 mix) ethoxysulphate (3 ethoxy groups)
C28AE	Alkyl (C12-C18 mix) ethoxylate
CDV	Critical dilution volume
ChF	Characterisation factor
CMC	Carboxymethyl cellulose
DF	Degradation factor
DID	Detergent Ingredient Database
EDTP Ca/Na salt	Ethylene diamine tetra methylene phosphonic acid Ca/Na salt
GFF	Grenelle frame formulations
HEDP	Etidronic acid
HERA	Human and environmental risk assessment
LAS	Linear alkyl benzenesulphonate, Na salt
LF	Loading factor
PEI ethoxylate	Polyethyleneimine ethoxylate
SDPP	Sodium diethylenetriamine pentamethylene phosphonate
STIWA	Stiftung Warentest
TF	Toxicity factor

1 Introduction

1.1 Toxicity in LCA

Ecotoxicity and human toxicity indicators remain of interest in life cycle assessment (LCA) studies. Since the first attempt to develop an ecotoxicity indicator in 1992 by the Centre voor Milieukunde Leiden (Heijungs et al. 1992) up to the ReCiPe approach in 2009 (Goedkoop et al. 2008), the latest one in the impact assessment methodology family, (eco)toxicity models were continuously improved including fate and exposure components. Toxicity assessment by means of LCA, with its underlying 'less is better' concept, has always been a complex and somewhat controversial task. LCA integrates emissions over time and space, which are very different from risk assessment, which compares exposure versus a toxicity threshold for a given temporal and geographical context. Validation of the exposure models by means of monitoring is not possible in LCA. Furthermore, the functional unit approach of LCA is inconsistent with risk assessment approaches that are based on environmental exposure levels. Risk assessment and LCA therefore serve different purposes. In risk assessment, safety is assessed and information gaps are handled by using conservative approaches. In LCA, the focus is not on absolute ecotoxicity thresholds, but on a comparison of products/services using the best available average data. Gradually, the consensus has grown wherein both tools have their own value and uses, and they are rather complementary, as described in the conclusion of the EU fifth FP OMNIITOX project (Pant et al. 2004; Pennington 2004).

1.2 Development of the critical dilution volume

Critical dilution volume (CDV) was originally developed as an evaluation criterion for detergent ingredients in the context of the European Eco-label scheme (EU Eco-label 1995). The CDV method uses the dimension of "litres per functional unit", which expresses the amount of water needed for the hypothetical dilution of a chemical substance to a safe level. To comply with the EU Eco-label requirements, the CDV of a product must not exceed an arbitrarily defined maximum value, and therefore uses an additive approach of ecotoxicity (Eskeland and Svanes 2004). This type of CDV calculation based on a defined functional unit can be applied more widely to provide a simple screening level tool for comparative product evaluations (Nitschke et al. 2007). For example, the Stiftung Warentest, a German consumer organization, compares detergents by use of the CDV approach.

To support the CDV calculation, a public source of agreed ecological data for detergent product ingredients was made available on the Detergent Ingredient Database List (or DID list). The DID list (DID list Part B 2004; DID list 2007) enables a comparative and transparent product evaluation for CDV calculations. On behalf of the EU Commission, the DID list was revised in 2004. The revision aimed to expand and update the database for detergent ingredients and to define a new set of CDV parameters. Although CDV calculations provide a quantitative assessment based on ecotoxicity data, the result is not equivalent to an environmental risk assessment. CDV can be considered as a product-based relative assessment based on the use of a functional unit (i.e. dose per wash), while environmental risk assessment provides a chemical-based absolute assessment based on specific exposure data and tonnages, which is the preferred approach for safety and regulatory management of chemicals (e.g. Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)).

1.3 Development of USEtox

The USEtox^{TM} model (Rosenbaum et al. 2008) is an advanced environmental model for characterization of human and ecotoxicity impacts for life cycle impact assessment and for the comparative assessment and ranking of chemicals according to their inherent hazard characteristics. It has been developed by a team of researchers from

the Task Force on Toxic Impacts under the UNEP-SETAC Life Cycle Initiative, and is positioned as a "consensus" model. This is, to our knowledge, the first model for which there is (1) a published list of about 3,000 characterisation factors for industrial chemicals, and 2) an easy to use tool for users to calculate or revise characterisation factors for chemicals of interest.

1.4 USEtox and the French "Grenelle" law on consumer environmental information

The fact that USEtox is positioned as a consensus model, involving scientific experts from multiple disciplines (Hauschild et al. 2008) makes it attractive to many users for assessing potential ecotoxicity impacts in LCA studies. It is, for example, being considered as the ecotoxicity method of choice for the French "Grenelle" Legislation. The "Grenelle de l'Environnement" is a project of law in which it is mentioned that sharing of environmental information for mass market products to consumers in France will be experimented at the point of sale. The in-market experimentation phase will begin on 1 July 2011 and will last at least 1 year and was preceded by some category pilot projects. After the experimentation phase, the French parliament will assess the opportunity to generalise this information (Cros et al. 2010).

In the 'Grenelle' pilot projects, the USEtox model has been proposed to assess the ecotoxicity impacts of several product categories (e.g. detergents, shampoos). Alternative options such as the CDV method were also considered. However, it was not possible to apply the USEtox method directly to the Grenelle pilot categories of detergents and shampoos, since even with ca. 3,000 chemicals listed, less than 50% of the mass of these types of product's ingredients were included. Secondly, the underlying models are complex, and the robustness and consistency of the results could not be validated. By contrast, for the CDV method, the DID lists allowed for a fast and unequivocal use for the detergent category.

1.5 Purpose of the paper

The purpose of this paper is to present the results of a side-by-side comparison of the USEtox and CDV methods which were conducted independently by Proctor & Gamble (P&G) and Unilever for three formats of detergent products. The aim of the work was to compare the relative ranking of the three detergent products with the two methods in order to better understand the advantages and limitations of each method. In this paper, we will report on the observations from the P&G "Grenelle" detergent pilot project and the Unilever detergent products comparisons, and propose the development of a list of representative USEtox characterisation factors (ChFs) for use in future detergent LCA studies.

2 Materials and methods

2.1 Scope

The P&G and Unilever case studies both involved the assessment of three laundry product formats, i.e. a powder, a dilute liquid and a concentrated liquid, with one based on market average formulations and one of actual producer formulations. The P&G case study used average frame formulations prepared by the French detergent industry based on information of representative laundry formulations for the French market. These Grenelle detergent frame formulations (GFF) were evaluated by P&G for the purpose of this paper and hence do not represent P&G formulations only. They had dosages of 85, 122 and 39 g for powder, dilute liquid and concentrated liquid, respectively. The Unilever assessment was conducted on Unilever product formulations, with dosages of 85, 113 and 37 g for powder, diluted liquid and concentrated liquid, respectively.

After use in a washing machine, the model agreed in the pilot phase of the Grenelle work assumed that the chemicals in these laundry products were disposed via the drain to a sewage treatment plant. Previous studies (Saouter et al. 2002; Van Hoof et al. 2003; Pant et al. 2004; Dewaele et al. 2006) have shown that, as far as freshwater ecotoxicity impacts are concerned, the disposal stage is the most important in the life cycle of detergents. For this reason, and to simplify the life cycle, the system boundary included only the discharge of the ingredients to the aquatic environment, after sewage treatment has taken place. Impacts of the treatment itself (e.g. energy, chemicals, infrastructure, etc.) as well as those from sludge disposal are excluded (Fig. 1), although any removal of the

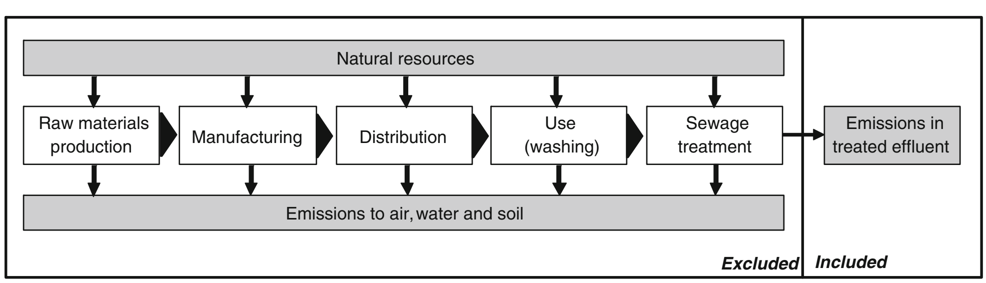

Fig. 1 System boundaries for the case studies

chemicals during treatment is included as part of the inventory modelling. The loading factor (LF) used in the 1999 version of the DID list (European Commission 1999) was used to calculate remaining ingredients in the effluent of the sewage treatment plant. The LF takes into account total removal in a sewage treatment plant, with sorption and biodegradation as the most important removal mechanisms for the chemicals involved (Eskeland and Svanes 2004). Rather than a full LCA, these system boundaries therefore correspond to an impact assessment of the laundry products at their end-of-life stage, focusing on freshwater ecotoxicity at the mid-point level, using CDV and USEtox as impact assessment methods. The functional unit is the amount of product required for one standard wash (Tables 1 and 2).

2.2 Critical dilution volume

Following the EU Eco-label approach a critical dilution volume was calculated for each ingredient (i) in the product according to Eq. 1. The new DID list (DID list 2007) now refers to a degradation factor (DF) which only considers elimination by biodegradation in surface waters. Therefore, other removal mechanisms such as adsorption onto sludge

Table 1 Dosage and composition of the three GFF products

	CAS	DID list no.	Regular powder	Dilute liquid	Concentrated liquid
Dosage per wash (g)			85	122.4	38.6
Composition			%	%	%
Water			7.80225	74.425925	45.587625
Sodium carbonate	497-19-8	122	22.175	–	–
Sodium sulphate	7757-82-6	133	19.8925	–	–
Sodium percarbonate	15630-89-4	127	13.275	–	–
Na, linear alkylbenzene	68411-30-3	1	8.69	5.0175	14.42735
Sulphonate	1318-02-1	114	7.0425	–	–
Zeolite	1344-09-8	124	4.7125	–	–
Sodium silicate		121	4.4825	–	–
Bentonite	10543-57-4	8	3.0875	4.58	–
C12-15 alkylethoxysulphate (3EO)	79-10-7	128	2.825	–	–
Tetra acetylethylene diamine	9004-32-4	NA	1.4835	–	–
(TAED)	77-92-9	132	1.2325	–	–
Sodium acrylic acid	97-54-1	115	0.9975	–	–
Carboxymethyl cellulose	107-75-5	142	0.7625	0.5375	1.3345
Citric	9003-44-7	116	0.575	–	–
Perfume	3794-83-0	119	0.535	0.4675	0.44975
Polycarboxylate polymer	9000-90-2	141	0.34825	0.3365	1.27975
Phosphonate (HEDP)	7647-14-5	134	0.0725	–	–
Enzymes	1103-38-4	143	0.0085	0.001075	0.001275
Sodium chloride	9004-82-4	8	–	3.205	6.11975
Dye	629-25-4	15	–	2.8815	6.035
C12 alkylethoxysulphate (3EO)	57-55-6	174	–	2.3575	6.713
Palm/kernel fatty acids	68-04-2	115	–	2.2225	3.4245
Propylene glycol	64-17-5	129	–	1.5525	–
Citrate	7775-19-1	NA	–	0.665	0.42
Ethanol	27306-79-2	28	–	1.75	12.1325
Metaborate	56-81-5	112	–	–	1.2425
C12-18 alkylethoxylate	68130-99-4	196	–	–	0.7475
Glycerine	27344-41-8	150	–	–	0.085
Polyethyleneimine ethoxylate polymer					
Biphenyl disulphonate					

NA not applicable

Table 2 Dosage and composition of the three Unilever laundry products

Dosage per wash (g)	CAS	DID list no.	Regular powder 85	Concentrated liquid 37	Dilute liquid 113
Composition					
Water		NA	X	X	X
Sodium carbonate	497-19-8	122	X	–	–
Sodium sulphate	7757-82-6	133	X	–	X
Sodium percarbonate	15630-89-4	127	X	–	–
Na, linear alkylbenzene sulphonate	68411-30-3	1	X	X	–
Zeolite	1318-02-1	114	X	–	–
Sodium silicate	1344-09-8	124	X	–	–
Bentonite		121	X	–	–
C12-15 alkylethoxysulphate (3EO)	10543-57-4	8	-	–	–
Tetra acetylethylene diamine (TAED)	79-10-7	128	X	–	–
Sodium acrylic acid	9004-32-4	NA	–	–	–
Carboxymethyl cellulose	77-92-9	132	–	–	–
Citric	97-54-1	115	X	–	–
Perfume	107-75-5	142	X	X	X
Polycarboxylate polymer	9003-44-7	116	–	–	–
Phosphonate (HEDP)	3794-83-0	119	X	X	X
Enzymes	9000-90-2	141	X	X	X
Sodium chloride	7647-14-5	134	X	–	X
Dye	1103-38-4	143	X	X	X
C12 alkylethoxysulphate (3EO)	9004-82-4	8	–	–	–
Palm/kernel fatty acids	629-25-4	15	X	X	X
Propylene glycol	57-55-6	174	–	X	X
Citrate	68-04-2	115	–	X	–
Ethanol	64-17-5	129	–	–	–
Metaborate	7775-19-1	NA	–	–	–
C12-18 alkylethoxylate	27306-79-2	28	–	–	–
Glycerine	56-81-5	112	–	X	X
Polyethyleneimine ethoxylate polymer	68130-99-4	196	X	X	–
Biphenyl disulphonate	27344-41-8	150	–	X	X
1,2-Benzisothiazol-3-one	2634-33-5	80	–	–	–
C12/15 A, 2–6 EO	68131-39-5	25	X	X	X
C12/14 Alkyl sulphate	9004-82-4	5	–	X	X
FWA 1		149	X	–	–
Block polymers	9010-92-8	196	X	X	–
Silicon	8050-81-5	110	X	–	–
Perborates		126	–	X	X
Starch	9005-25-8	144	X	–	–
Glyceryl stearate	31566-31-1	185	X	–	–
C14/17 Alkyl sulphonate	16090-02-1	3	X	–	–
Xanthan gum	11138-66-2	189	X	–	–
Hydroxethyl laurdimonium chloride	85736-63-6	NA	–	–	X

NA not applicable

X ingredient used in the formulation

or precipitation are no longer included. The toxicity factor (TF) should ideally be calculated using chronic toxicity data and chronic safety factors. However, if there are no chronic test results available, then acute toxicity data and safety factors must be used. The chronic toxicity factor ($TF_{chronic}$) is the lowest median of the

trophic levels calculated.

$$\mathrm{CDV}_i \equiv w_i \times \mathrm{DF}_i \times \frac{1,000}{\mathrm{TF}_{\mathrm{chronic}_i}}, \quad (1)$$

where w_i is the weight of substance i in the effluent per functional unit (in grammes), DF_i is the surface water degradation factor for substance i as defined in the EU DID list (unitless) and $\mathrm{TF}_{\mathrm{chronic}_i}$ is the chronic toxicity factor for substance i as defined in the EU DID list (milligrammes per litre).

The product's CDV score is then calculated by adding the CDVs of the individual ingredients multiplied with their dosage per wash, assuming full additivity of the ecotoxicity. If there were data gaps in the DID list, then analogous substances were selected, or the CDV was calculated directly using available ecotoxicity data, details provided in Tables 3 and 4.

2.3 USEtox

USEtox (Rosenbaum et al. 2008) is a novel and rather sophisticated method to calculate the hazard of a substance i, taking into account its toxicity (ecological effect factor), its fate in several environmental compartments (fate factor) and its exposure (exposure factor). The combination of these three factors leads to a characterization factor (in potentially affected fraction (PAF) cubic meter day per kilogramme) for a specific substance i, emitted to a given environmental compartment. The product's freshwater ecotoxicity score is then calculated using Eq. 2.

$$\mathrm{FW}_{\mathrm{ecotox}} \equiv \sum_{i=1}^{n} (w_i \cdot \mathrm{ChF}_i), \quad (2)$$

where w_i is the weight of substance i in the effluent per functional unit (in kilogrammes), ChF_i is the USEtox freshwater ecotoxicity characterization factor for substance i (PAF cubic metre day per kg) and $\mathrm{FW}_{\mathrm{ecotox}}$ is the product's freshwater ecotoxicity (PAF cubic metre day).

A published list of ChFs for approximately 3,000 organic chemicals (USEtox Development Team 2010) includes some data for laundry ingredients. For the three GFF and the Unilever detergent calculations, only self-calculated ChFs were used as listed in Tables 3 and 4.

For the GFF, input data for the calculation of USEtox ChF were primarily derived from published Human and Environmental Risk Assessments (HERA) on detergent ingredients (AISE and CEFIC 2010), the USEPA Ecotox database (USEPA 2010), the EPI Suite experimental database and estimation programmes (USEPA 2009a), as well as P&G internal data. For the Unilever products, the following sources were used: the EPI Suite experimental database and estimation programmes (USEPA 2009a), HERA studies (AISE and CEFIC 2010), IUCLID datasheets (European Commission 2010), the ChemIDplus database (U.S. National Library of Medicine 2010), the Hazardous Substances Data Bank (U.S. National Library of Medicine 2009), the USEPA Ecotox database (USEPA 2010), Unilever internal data and Ecosar estimation programme (USEPA 2009b). The latter source was only used in cases where no experimental ecotoxicity data at all were available (five chemicals only). In the Electronic Supplementary Material, the detailed substance-specific data used and sources are shown.

Since perfume is a complex mixture of different chemicals, it was assumed for the GFF that a perfume is composed of ethanol, isoeugenol and hydroxycitronellal (40/30/30 by mass). These ingredients were selected as they are commonly present in laundry perfumes and all have sufficient environmental data, which are the necessary input for USEtox. With this assumption, it was possible to calculate a USEtox 'perfume' ChF by taking the individual perfume chemical USEtox ChFs and weighting them according to their assumed proportions. For the Unilever perfume ChF, a more detailed composition for the perfume was obtained from a material safety datasheet, and ChFs were calculated for the individual chemicals. A weighted ChF was then calculated for the perfume. However, as the perfume's composition was given as concentration ranges rather than exact concentrations, this added a level of uncertainty to the weighted ChF. For both case studies, the uncertainty (due to assumptions or lack of data availability) on the perfume ChF is considered acceptable, since the primary purpose of this paper is to evaluate product ranking, thus a relative comparison and not an absolute assessment (pass/fail criterion) was done, as opposed to the EU Eco-label.

In general, obtaining quality data to satisfy the demand of the USEtox model proved to be very challenging for both P&G and Unilever. Experimental values for some physical–chemical properties were not available and had to be estimated using the estimation programmes from EPI Suite. In the particular case of degradation rates, in most cases the EPI Suite had to be used. Despite the effort in data collection, there were 12 chemicals in the Unilever products from which no factors could be calculated due to the lack of data for one or more parameters. As a consequence, these 12 chemicals were excluded from the impact assessment. These chemicals constituted less than 10% in weight in all three products.

A particular case to be highlighted is that of inorganic chemicals, such as sodium percarbonate, sodium chloride,

Table 3 Overview of DID list values and USEtox environmental characterization factor for a GFF emission to the freshwater compartment

	DID list number	LF	DF –	$TF_{chronic}$ mg/L	USEtox FW ecotoxicity characterization factor PAF m^3 day kg^{-1}
Sodium carbonate	122	0.8	0.15	0.25	8.5E+02
Sodium sulphate	133	1	1	1	7.6E+01
Sodium percarbonate	127	0.8	0.15	0.25	2.6E+02
Na, linear alkylbenzene sulfonate	1	0.05	0.05	0.069	2.6E+00
Zeolite	114	0.05	1	3.5	4.6E+02
Sodium silicate	124	0.8	1	0.25	3.1E+02
Bentonite[a]	121	0.05	1	1	4.6E+02
C12-15 alkylethoxysulphate	8	0.03	0.05	0.01	3.3E+02
(3EO)[b]	128	0.13	0.05	5	1.6E+01
Tetra acetylethylene diamine	NA	0.13	0.05	0.41	2.0E+02
(TAED)	132	0.75	0.5	0.05	1.0E+00
Sodium acrylic acid[c]	115	0.07	0.05	1.6	2.2E+01
Carboxymethyl cellulose	142	0.1	0.5	0.002	7.1E+02
CITRIC acid[c]	116	0.4	1	10.6	3.9E+02
Perfume	119	0.4	1	0.5	4.6E+03
Polycarboxylate polymer	141	0.13	0.05	0.005	7.2E-01
PHOSPONATE (HEDP)	134	1	1	1	3.1E+01
Enzymes	143	0.4	1	0.01	4.6E+03
Sodium chloride	8	0.03	0.05	0.01	7.6E+01
dye (CI 15630)	8	0.03	0.05	0.01	5.9E+02
C12 alkylethoxysulphate (3EO)	15	0.05	0.05	0.1	3.2E+01
C15 alkylethoxysulphate (3EO)	174	0.13	0.05	0.1625	1.3E-01
Palm/kernel fatty acids	115	0.07	0.05	1.6	2.6E+00
Propylene glycol	129	0.13	0.05	1	2.2E-01
Sodium citrate[c]	NA	1	1	0.014	6.4E+02
Ethanol	28	0.03	0.05	0.0035	1.4E+02
Metaborate	112	0.13	0.05	0.88	2.3E+00
C12-18 alkylethoxylate[c]	196	1	1	0.02	3.1E+02
Glycerine	150	0.4	1	0.1	7.8E-01
polyethyleneimine ethoxylate polymer					
Biphenyl disulphonate					

NA not applicable

[a] Assumed same as zeolite for USEtox calculation

[b] Average value for C12 and C15 AE3S

[c] Data are from the published list of USEtox characterization factors for organics (v1.01)

[d] Assumed alkyl (C14) ethoxylate (7 ethoxy groups)

or sodium silicoaluminate, which are common ingredients in laundry products, especially powders. USEtox is mainly designed to model organic chemicals, since environmental partitioning is based on parameters like K_{ow} and K_{oc} which are not measured for inorganic chemicals. In the absence of better data and to obtain a ChF, the approach taken to calculate ChFs for these chemicals was to set to zero ($1 \times e^{-20}$ in the spreadsheet) for the following parameters: K_{ow}, K_{oc}, vapour pressure and all degradation rates. This approach was accepted by the USEtox team as a first approximation, as far as the freshwater compartment is concerned (Huijbregts 2010).

Tables 3 and 4 show the ChFs obtained by P&G and Unilever, respectively, and Tables 1 and 2 in the Electronic Supplementary Material provide an overview of the input values used for the USEtox ChF calculations.

Table 4 Overview of DID list values and USEtox environmental characterization factor for an emission to the freshwater compartment in the Unilever case study

Name	DID list number	LF	DF	$TF_{chronic}$	USEtox FW ecotoxicity characterization factor
		–	–	mg/L	PAF m^3 day kg^{-1}
Alpha-isomethyl ionone	142	0.1	0.50	0.002	5.89E+03
Aluminium silicate	124	0.8	1.00	0.25	7.99E+01
Amylase	141	0.13	0.05	0.005	1.31E+02
Aqua		1	1.00		0.00E+00
Benzisothiazolinone	80	0.6	0.50	0.00015	6.24E+03
Butylphenyl methylpropional	142	0.1	0.50	0.002	9.91E+03
C12-15 Pareth-5	25	0.03	0.05	0.0036	4.51E+02
C12-15 Pareth-7	25	0.03	0.05	0.0036	4.51E+02
Cellulose gum	132	0.75	0.50	0.05	No data
CI 11680	143	0.4	1.00	0.01	No data
CI 12490	143	0.4	1.00	0.01	No data
CI 19140	143	0.4	1.00	0.01	6.36E+00
CI 42051	143	0.4	1.00	0.01	No data
CI 42090	143	0.4	1.00	0.01	1.27E-03
CI 45100	143	0.4	1.00	0.01	2.04E+00
CI 61585	143	0.4	1.00	0.01	No data
Citric acid	115	0.07	0.05	1.6	3.87E+01
Citronellol	142	0.1	0.50	0.002	1.17E+03
Dimorpholinopyridazinone	149	0.4	1.00	0.1	No data
Disodium distyrylbiphenyl disulphonate	150	0.4	1.00	0.1	8.53E-01
Ethylene diamine tetra methylene phosphonic acid Ca/Na salt	119	0.4	1.00	0.5	2.35E+03
Formyl phenyl boronic acid	126	1	1.00	0.014	2.39E+03
Geraniol	142	0.1	0.50	0.002	7.21E+03
Glycerin	112	0.13	0.05	0.88	1.14E+00
Glyceryl stearate	185	0.07	0.05	0.02	6.54E+01
Hydroxyethyl laurdimonium chloride[a]	SC	0.13	0.05	0.001	No data
Maize starch	144	0.1	0.05	0.1	No data
Perfume[b]	142	0.1	0.50	0.002	1.24E+04
Polyethylene terephthalate	196	1	1.00	0.02	No data
Polyoxymethylene melamine	196	1	1.00	0.02	No data
Propylene glycol	174	0.13	0.15	32	1.43E+02
Protease	141	0.13	0.05	0.005	7.07E+03
Simethicone	110	0.4	1.00	0.25	4.01E+01
Sodium bentonite	121	0.8	1.00	1	7.99E+01
Sodium carbonate	122	0.8	0.15	0.15	4.37E+02
Sodium carbonate peroxide	127	0.8	0.15	0.15	2.15E+02
Sodium chloride	134	1	1.00	1	3.33E+01
Sodium citrate	115	0.07	0.05	1.6	2.38E+01
Sodium diethylenetriamine pentamethylene phosphonate	119	0.4	1.00	0.5	1.10E+02
Sodium dodecylbenzenesulfonate	1	0.05	0.05	0.069	3.45E+02
Sodium laureth sulphate	5	0.02	0.05	0.02	4.00E+02
Sodium palm kernelate	15	0.05	0.05	0.1	2.93E+02
Sodium polyaryl sulfonate	149	0.4	1.00	0.1	1.11E+02
Sodium silicate	124	0.8	1.00	0.25	4.42E+02
Sodium Silicoaluminate	114	0.05	1.00	3.5	7.99E+01
Sodium stearate	15	0.05	0.05	0.1	3.77E+01

Table 4 (continued)

Name	DID list number	LF	DF	$TF_{chronic}$	USEtox FW ecotoxicity characterization factor
		–	–	mg/L	PAF m^3 day kg^{-1}
Sodium sulphate	133	1	1.00	1	2.95E+01
Sorbitol	112	0.13	0.05	0.88	5.87E-03
Stearic acid	15	0.05	0.05	0.1	4.47E+01
Styrene/acrylates copolymer	196	1	1.00	0.02	No data
TEA-cocoate	15	0.05	0.05	0.1	No data
Tetraacetyl ethylene diamine	128	0.13	0.05	5	1.26E+01
Tetrasodium Etidronate	119	0.4	1.00	0.5	2.85E+02
Xanthan gum	189	0.13	0.05	0.49	3.59E+01

[a] There is no DID list value for hydroxyethyl laurdimonium chloride, and so the DF and TF were calculated based on internal data

[b] USEtox factor calculated as weighted average from the following composition of chemicals: 2,6-dimethyloct-7-en-2-ol (50%), hexyl salicylate (20%), 2-(4-tert-butylbenzyl)propionaldehyde (10%), 2,6-di-tert-butyl-p-cresol (10%), benzyl acetate (9%), dodecan-1-ol (1%)

SC self-calculated

3 Results

3.1 Critical dilution volume

Figures 2 and 3 show the CDV results for the GFF and Unilever product formulations, respectively. The dilute liquid product was selected as the reference, since it had the highest CDV score. For the GFF, the powder and concentrated liquid scores were 19% and 22% lower, respectively. For the equivalent Unilever product formulations, the results were 33% and 67% lower. Both figures show the ingredients which contributed to at least 1% of the total product scores, and all other ingredients were classified as part of the "other" category. Tables 3 and 4 provide the CDV input values for the various detergent ingredients.

3.2 USEtox

Figures 4 and 5 show the USEtox results for the GFF and Unilever product formulations, respectively. In this case, the powder product was selected as the reference since it had the

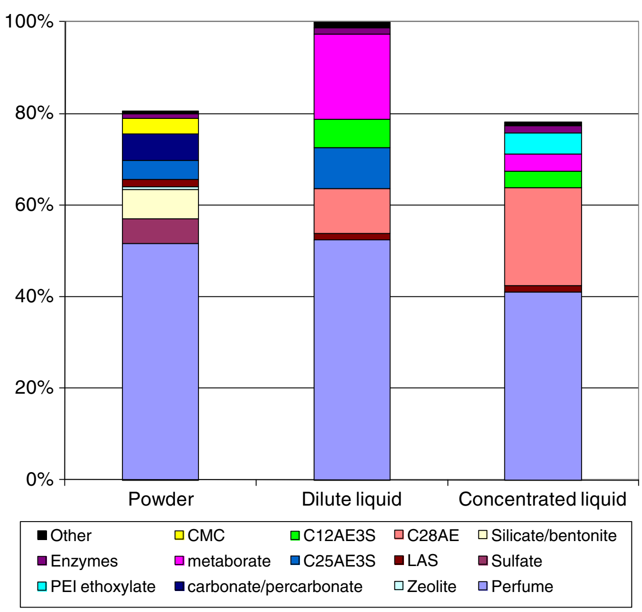

Fig. 2 Comparison of three GFF using the critical dilution volume. Results are for one wash relative to dilute liquid

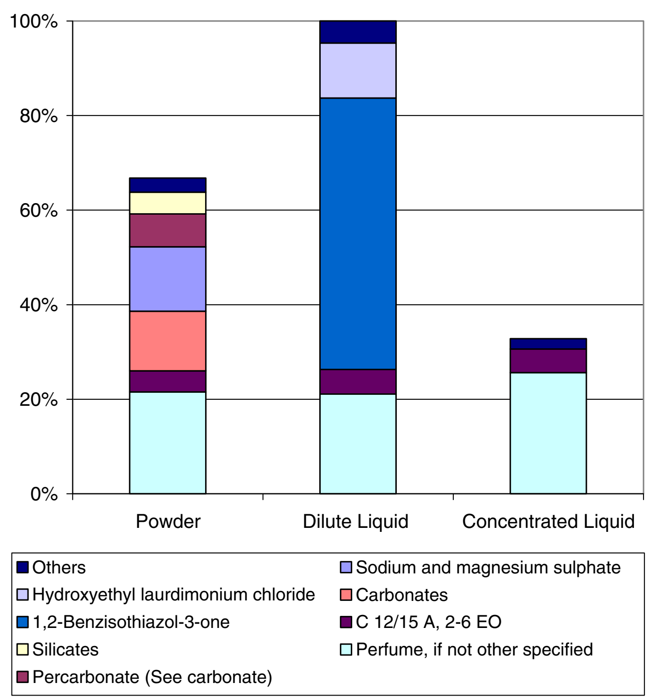

Fig. 3 Comparison of three Unilever laundry products using the critical dilution volume. Results are for one wash and relative to dilute liquid

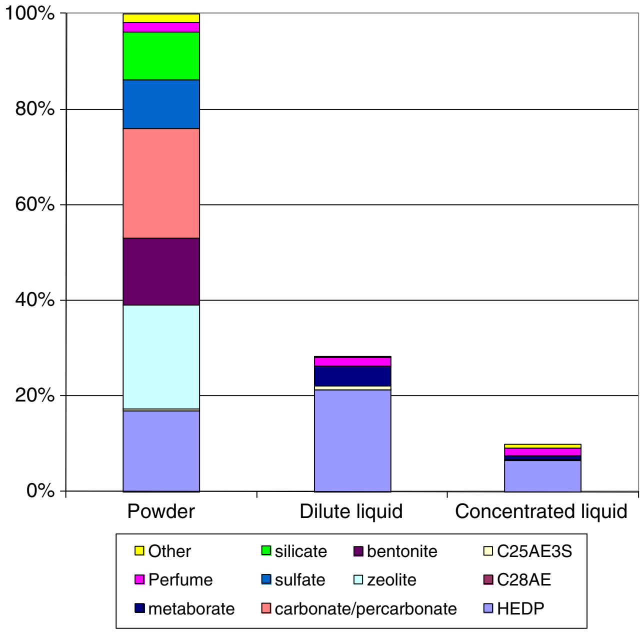

Fig. 4 Comparison of three GFF using the freshwater ecotoxicity characterization factors from USEtox. Results are for one wash relative to powder

highest USEtox score. For the GFFs, the dilute and concentrated liquid scores were 72% and 90% lower, respectively. For Unilever, the equivalent products were both 90% lower. Both figures also show the ingredients which contributed to at least 1% of the total product scores; ingredients contributing less than 1% were classified as part of the “other” category.

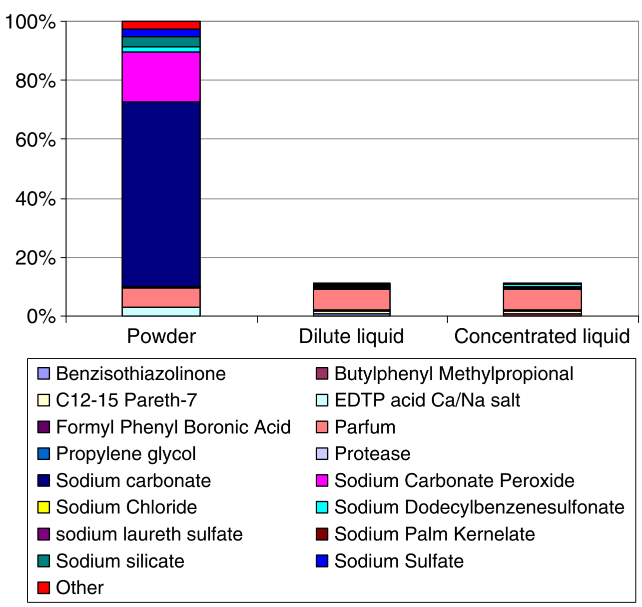

Fig. 5 Comparison of three Unilever laundry products using the freshwater ecotoxicity characterization factors from USEtox. Results are for one wash relative to powder

3.3 Default USEtox vs. self-calculated ChFs

A comparison was also made between the USEtox freshwater ecotoxicity ChFs as published in the list of organic materials and those recalculated by P&G and Unilever (Figs. 6 and 7). In total, nine and 15 ingredients were independently recalculated by P&G and Unilever, respectively. The difference with the default ChFs are shown in orders of magnitude. For the P&G assessment, all self-calculated ChFs were consistently lower by up to three orders of magnitude. For the Unilever assessment, the difference may be as great as five orders of magnitude, although overall there is a better match with the published (default) values. Absolute values are listed in the Electronic Supplementary Material.

4 Discussion

4.1 Input data

USEtox has a database with ChFs for about 3,000 substances, and yet this was insufficient for the present study, and many additional ChFs had to be calculated for missing substances or for missing isomers/homologues. For comparison, the DID list used in the CDV approach contains around 200 ingredients. However, this list has been specifically developed for laundry products so that ingredient gaps are obviously less common than in USEtox for detergent ingredients.

One of the main advantages of the USEtox method is its comprehensive fate and effects modelling, but this comes at a price, namely the effort in data collection required when new ChFs have to be calculated. We estimated that on average, data collection and review for freshwater ecotoxicity ChFs typically requires around 1 h per substance.

Fate modelling in USEtox—as in the most commonly used models in risk assessment such as EUSES (EUSES 2008)—is based on fugacity modelling, and this is designed to predict the fate of organic chemicals rather than inorganic chemicals. However, in the case of laundry products, inorganic chemicals are common ingredients, and yet it is not clear to what extent USEtox can be used to model such chemicals. Using quantitative structure–activity relationships (QSAR) estimations for inorganic chemicals and also large polymers may result in unreliable outcomes. An additional problem, for organic and inorganic chemicals, is that there are not enough experimental data to cover all the required parameters in the fate model, which leads to an extensive use of QSAR estimations. It would be useful if the USEtox manual could provide more guidance on how to address these issues.

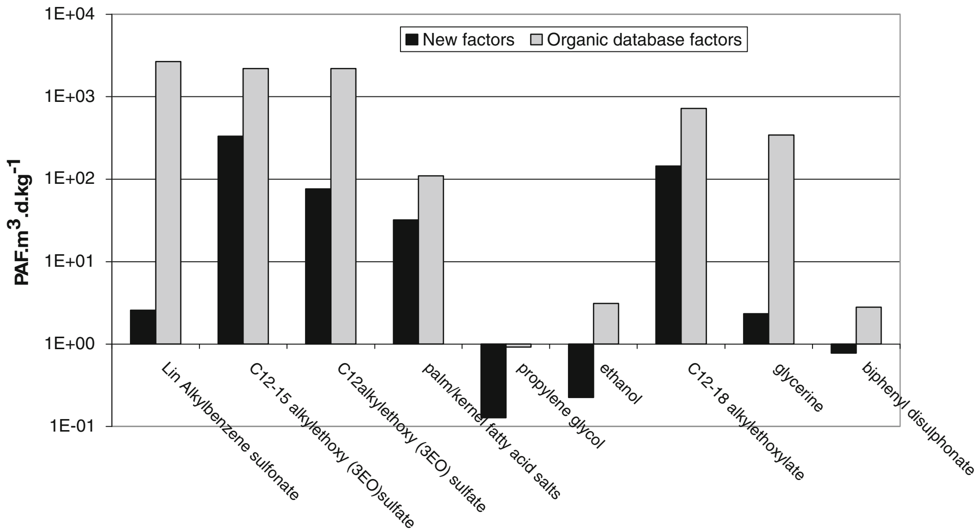

Fig. 6 Comparison of USEtox freshwater ecotoxicity characterization factors from the published list with P&G calculated values. Differences are shown in orders of magnitude

4.2 Product ranking with CDV

Even though the GFF are different from the Unilever product formulations, the ranking of the three detergent formats using the CDV method is similar (see Figs. 2 and 3). Liquid dilutes have the highest CDV value and powders are similar to concentrated liquids, although in the Unilever case study, concentrated liquid has a lower score than powder. Perfume is consistently the most important ingredient contributing approximately 20% or higher of the total score, except for Unilever's dilute liquids format, where the most important is the preservative 1,2-benzisothiazol-3-one. In powder formats, inorganic chemicals (including carbonates, sulphates, silicates and zeolites) are responsible for the majority of the remaining score, whereas for liquid formats surfactants both organic and inorganic chemicals (metaborate) are important. As inorganic chemicals are by definition not biodegradable, the CDV impact method does not include removal of these chemicals in surface water, which is unrealistic for some of them.

4.3 Product ranking with USEtox

The ranking based on USEtox using self-calculated ChFs is similar for the GFF and the Unilever products. Powder formats have the highest score followed by dilute liquids and concentrated liquids. This illustrates that the specific composition of the detergent formulation per product type is less important in determining the ranking than the conceptual differences between the two assessment methods. It also shows that the different approach on perfume (see Section 2.3) is not of importance for the relative ranking.

For powder, the inorganic compounds are mainly driving the total score (see Figs. 4 and 5) for both the GFF and Unilever product. For liquid products, the most important contributors to the USEtox score is phosphonate (HEDP)

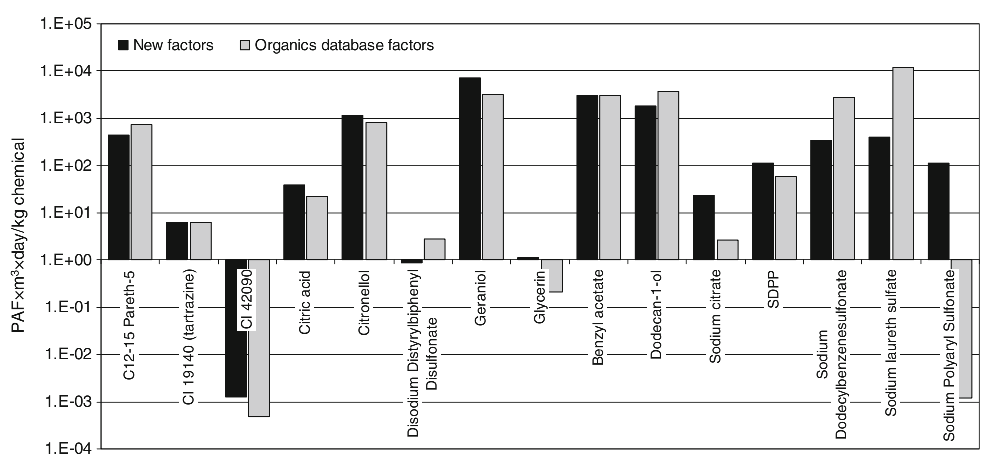

Fig. 7 Comparison of USEtox freshwater ecotoxicity characterization factors from the published list with Unilever calculated values. Differences are shown in orders of magnitude

for the GFF, whereas for the Unilever products, perfume and surfactants are the most important.

It is interesting that inorganic ingredients rank higher with the USEtox method than with the CDV method. This explains their contribution in the powder product. The product comparison and influence of inorganic ingredients in the product score contribution is consistent with the observations made on IMPACT 2002 toxicity scores within the OMNIITOX project on the detergent case study (Pant et al. 2004). The high contribution from inorganic chemicals with IMPACT 2002 was attributed to residence time in the water column (lakes). Again, in line with the OMNIITOX detergent case study, the high ChFs for some common inorganic chemicals obtained with USEtox can be questioned for their environmental relevance, and they are likely to be an artefact of their persistent-like behaviour within the model.

4.4 Default vs. self-calculated USEtox ChFs

With the launch of the USEtox model, a list of ChFs for ~3,000 organic substances was available for download. This list contained some ingredients commonly used in laundry detergents, e.g. some surfactants. Within the risk assessment, work done in HERA (AISE and CEFIC 2010) and more recently with the REACH first registration deadline, data for high-volume chemicals were extensively reviewed in terms of their quality. ChFs for relevant chemicals were therefore recalculated and compared to the USEtox published values to assess the accuracy of the latter. This was done independently by P&G for the chemicals used in the GFF (see Fig. 6) and by Unilever for their products (see Fig. 7).

For the GFF, there were nine ingredients with published ChFs. A trend was observed that self-calculated ChFs were always lower (up to three orders of magnitude) than the published values. Although the actual data sources for each substance are not disclosed in the database, a reason for this discrepancy could be that for the calculation of the first 3,000 chemicals QSARs were used to populate the list within a reasonable time period (avoiding extensive literature research). The values in the published USEtox list could therefore be seen as conservative screening values and not definitive values. It can be expected that for the calculation of the freshwater ecotoxicity, water solubility (Sol25), the first order degradation rate constant in water ($kdeg_W$) and the ecotoxicity value ($av_{logEC50}$) are the most important parameters in deriving ChFs. The self-calculated input parameters vary by 5, 3 and 4 log units, respectively compared to the respective input parameters in the published list of ChFs. Since the ChF is inversely proportional to each of them, the observed difference with the published values is largely explained by the differences in these values. In addition, some input parameters used for surfactants in the USEtox ChF calculation are highly dependent on the alkyl chain length and/or ethoxylation number (AISE 2004). Taking into account such refinements, the self-calculated USEtox freshwater ecotoxicity ChF for alkylethoxysulphate (AE3S) is one order of magnitude lower for the C12 alkyl chain length variant compared to the C15 variant (see Table 3). Furthermore, the description in the USEtox published list is not sufficiently detailed to discriminate surfactants homologies and isomers. This is an important issue if the USEtox method is intended for comparative purposes rather than to identify hotspots in the life cycle. Surfactant chain length is an important descriptor/discriminator in the DID list.

For the Unilever product formulations, the differences between the published and self-calculated ChF is less than one order of magnitude for 13 out of 15 chemicals. For these chemicals, the physical–chemical properties and degradation rates were primarily derived from EPI Suite data, and the HC50 values used were similar. However, for the surfactant sodium lauryl ether sulphate the difference is 1.5 orders of magnitude, and for the optical brightener, the difference between the ChFs is five orders of magnitude. The reason for these higher orders of difference is because different data sources are used, especially for physical–chemical properties and degradation rates. The self-calculated ChF for the optical brightener is based on data from the risk assessment published by HERA (AISE and CEFIC 2010), whereas the data sources in the USEtox database are not disclosed. A similar difference was observed by P&G, and in both cases higher tier risk assessment data were used as input data for determining the ChF. This illustrates the sensitivity of the ChF to different data sources, and there is a risk that different LCA practitioners in the absence of agreed published ChFs could obtain very different ChF values for the same chemical. This risk is lower if less data is available and practitioners rely on common QSAR models such as the EPI Suite.

4.5 Conceptual differences between CDV and USEtox

The different product rankings obtained with the two methods is confusing in a decision making context and is highly unsatisfactory for communication purposes such as product labelling.

USEtox and CDV methods were developed for different purposes, and a list of their advantages and drawbacks is provided in Table 5. CDV originated as a specific tool for the European Eco-label, whereas the USEtox method is a more generic tool, with the potential of assessing any product on a life cycle basis. Although CDV can be used to compare products, it must be highlighted that in the Eco-label scheme it is only used

Table 5 Advantages and drawbacks of USEtox and CDV for comparative assessment of laundry products

	USEtox	CDV
Advantages	• Harmonised and recognized in the LCA community	• Simple approach for chemicals on DID list
	• Potential scope is life cycle, not only disposal	• Already in use for EU Eco-label scheme
	• Comprehensive list of detergent ingredients	
	• Comprehensive fate and effects modelling	
	• Specifically built for comparing chemicals	
Drawbacks	• Insufficient substance coverage: ChFs have to be self-calculated	• Only for chemicals included in DID list
	• Data hungry: at least 12 variables per substance	• There is limited environmental fate modelling (only biodegradation)
	• Currently insufficient or poor data for many substances	• Heavily weighted against perfumes, preservatives, optical brighteners and dyes
	• Data collection is time consuming: ~1 h per substance	• Unrealistic approach for degradation and safety factors
	• Mainly designed for organic chemicals; not fully clear how to model inorganics	• Not designed to be protective of ecosystem structure and function
	• Not designed to be protective of ecosystem structure and function	• Unknown level of uncertainty
	• High level of uncertainty	

to assess whether a product exceeds a defined CDV threshold value. On the contrary, USEtox has been designed with the goal of comparing chemicals and this is reflected, for example, in the effect factor HC50, being based on a geometric mean of endpoints rather than on the most sensitive species data (Rosenbaum et al. 2008). The advantage of using the HC50 approach is that it can be calculated when there is poor data availability, typically three acute data values. However, the disadvantage of this approach is that it will not be protective of the most sensitive species, and therefore the focus has shifted away from the protection of the function and structure of ecosystems (Larsen and Hauschild 2007). This could be a potentially important drawback if a chemical is much more toxic to one trophic level of organisms (e.g. herbicides for algae). In contrast, the CDV approach is more conservative and protective of all trophic levels, with a focus on chronic toxicity and the flexibility to use higher safety factors depending on data availability. Consequently, the CDV TF is more closely aligned to the PNEC (predicted no-effect concentration) used in the environmental risk assessment.

The main advantage of the CDV method is that it is a simple approach, and it typically covers all the ingredients used in laundry products. However, the simplicity of the approach also becomes one of its main drawbacks, as listed in Table 5. This leads to proportional high contributions from inorganic materials because of simplistic fate models or assumptions and from perfumes, preservatives, optical brighteners and dyes (conservative safety factors for extrapolating acute to chronic toxicity (Nitschke et al. 2007)). Using total removal (instead of biodegradation only) in the fate model of CDV makes the CDV approach more relevant and consistent with USEtox, whilst keeping its benefit of simplicity. This approach is used for the evaluation of laundry products by the German Stiftung Warentest.

As explained in the introduction, it has become a common understanding that environmental risk assessment and ecotoxicity indicators in the life cycle impact assessment should be used for different purposes. Furthermore, it is possible that the ecotoxicity indicator in an LCA study could rank an individual product as preferable through the 'less is better' approach, even though it may contain ingredients which would not pass an environmental risk assessment threshold for a specific use scenario (i.e. due to difference between functional unit approach versus market tonnages). In addition, USEtox and CDV are both essentially hazard-based approaches, and they assume that ecotoxicological impacts are additive. However, this raises the issue of 'mixture toxicity': whether effects of individual ingredients will actually be synergistic, antagonistic or additive (ECETOC report 2001).

As an alternative to the hazard-based approach, the European Soap and Detergent Association (AISE), which represents the soaps, detergents and maintenance products industry in Europe, has developed the Environmental Safety Check (ESC) Tool. This is part of a voluntary initiative for companies to register their products for the Advanced Sustainability Profile status under AISE Charter 2010. The ESC tool is a risk-based system, using total EU industry tonnage information to provide a screening environmental risk assessment of individual ingredients in AISE products, which is consistent with the risk-based approach used for REACH (AISE Charter 2010).

4.6 Uncertainty

A common problem for both approaches is uncertainty. This is well documented in the case of USEtox, where a precision of two to three orders of magnitude is stated for human toxicity ChFs and one to two orders of magnitude for freshwater ecotoxicity (Rosenbaum et al. 2008). It must be taken into account that this accuracy estimation does not take into account potential errors in chemical-specific data, which can be high when QSAR estimations are used instead of experimental data. As for CDV, the level of uncertainty involved in the calculations is not reported, although the parameter uncertainty has the potential to be lower due to the lower complexity of the modelling.

The uncertainty issue raises an important question if the methods are intended for comparative purposes namely, how big must the differences be between alternative products in order to conclude that they are statistically significant? This type of question was addressed for a carbon footprint calculation of detergent products by de Koning et al (2010). In CDV, this aspect is unknown, and from the point of view of eco-labelling it is not relevant, as CDV is only used to check compliance with a dilution volume threshold. On the other hand, the question becomes important if CDV is to be used to compare alternative products, as it would be the case in the Grenelle initiative. In the case of USEtox, it is not clear if this model can be used to compare full products, since this potential application is not mentioned by Rosenbaum et al. (2008), who recommends instead its usefulness to identify the most critical 10–30 chemicals in a product system. However, if USEtox is to be used to compare ecotoxicity impacts for alternative products, the one to two orders of magnitude precision for individual substances must be taken into account and communicated. In Figs. 4 and 5, for example, it can be seen that the three product scores are within the same order of magnitude, implying that differences in impact score are unlikely to be significant. There is, therefore, a risk of misinterpretation, if initiatives like Grenelle assign single ecotoxicity scores to products without qualification of the level of significance. For instance, a consumer looking at the values presented in Figs. 4 and 5 would wrongly conclude the various products are different.

5 Conclusions

- Whilst risk assessment remains the most realistic and recommended method to address chemical safety, there is a growing interest to evaluate products on their comparative ecotoxicological properties. Three different detergent product formats were ranked using two commonly used ecotoxicity impact methods: the CDV approach used in the EU Eco-label and the USEtox freshwater ecotoxicity method. The relative ranking of the products with these two methods is inconsistent, for example, powder is most preferred by CDV and least preferred by USEtox. This is undesirable if the assessment is intended to inform consumers in their purchasing decisions such as currently being proposed in France.
- Addressing uncertainty is a critical issue if either the CDV or USEtox method is used to compare different laundry products. Uncertainty in CDV is not addressed at all, whereas in USEtox ChFs have an error of one to two orders of magnitude. This should be taken into account when interpreting impact scores, and we would conclude that there is no difference between the three product formats assessed.
- The different ranking of products can be attributed to the different underlying conceptual approaches of the CDV and USEtox methods.
- The inclusion of a comprehensive fate and multimedia exposure model for inorganic chemicals, in USEtox should in principle be more ecologically relevant than the CDV approach in the current EU Eco-label.
- CDV can be made more consistent with USEtox (and more relevant) if other removal mechanisms, besides surface water biodegradation, were included. In addition, the current algorithm does not account for removal in sewage treatment plants, which is not representative of the European context.
- It is shown that due to the extensive data input needs for the USEtox method, the resulting ChFs for freshwater ecotoxicity may differ by several orders of magnitude between different practitioners. Therefore, development of an industry agreed list of ChFs is recommended for commonly used ingredients. Data collection for obtaining new ChFs is a time-consuming task, which means that using USEtox on a regular basis in this kind of assessment is only feasible if chemical coverage is improved. Furthermore, high-quality experimental data for most chemicals are rather scarce, leading to an excessive use of QSAR estimations or in the worst case to the impossibility of calculating ChFs for some chemicals.
- The EU DID list discriminates some surfactants in terms of their alkyl chain length and/or ethoxylation number. Both of these descriptors have important effects on toxicity, which are not sufficiently documented in the published USEtox list of organic chemicals.
- Since inorganic chemicals are essential ingredients in laundry powders and their modelling is not adequately addressed in USEtox, as recognized by the developers,

this method is not yet ready for use within a product labelling context. Their proportionally high contribution in the USEtox ecotoxicity score for powders is difficult to interpret in terms of ecological relevance. This was also observed in the EU OMNIITOX project on detergents.

6 Recommendations and outlook

- There is a need for clear guidance and/or improved models for inorganic chemicals, which are commonly found in laundry products.
- In terms of data availability, not only data quantity, but also data quality, must be improved, something that has already been identified as a priority by the USEtox team (Rosenbaum et al. 2008). If less than three acute toxicity values are available, an interim factor could be published until better data are available through schemes such as REACH.
- CDV would benefit from taking into account sewage treatment removal in addition to environmental degradation, which was an additional consideration for this case study. Also, toxicity factors should be updated with the most recent data, such as HERA risk assessments (AISE and CEFIC 2010). Furthermore, the approach would benefit from developing environmental fate factors, although not necessarily with the level of sophistication in USEtox. Instead, the inclusion of fate based on independent key properties, as for example in the EDIP97method (Hauschild and Wenzel 1998) would be preferred, thus keeping the method simple, but not too simplistic.
- It is recommended to develop a list of USEtox ChFs for common detergent ingredients, in analogy with the EU DID list, to avoid different approaches for filling data gaps with USEtox input parameters, and a review procedure to officially introduce these revised values in the USEtox ChF list.

References

AISE & CEFIC (2004) Alcohol Ethoxysulphates (AES) Environmental risk assessment. Human & environmental risk assessment on ingredients of European household cleaning products. HERA Project, http://www.heraproject.com/RiskAssessment.cfm?SUBID=1. Accessed 17 Dec 2010

AISE & CEFIC (2010) Human and environmental risk assessment on ingredients of household cleaning products. http://www.heraproject.com/Index.cfm. Accessed 3 Dec 2010

AISE Charter (2010) Environmental safety check manual v1.0 (2010). http://www.sustainable-cleaning.com/en.companyarea_documentation.orb. Accessed 17 Dec 2010

Cros C, Fourdrin E, Réthoré O (2010) The French initiative on environmental information of mass market products. Int J Life Cycle Assess 15(6):537–539

De Koning A, Schowanek D, Dewaele J, Weisbrod A, Guinée J (2010) Uncertainties in a carbon footprint model for detergents; quantifying the confidence in a comparative result. Int J Life Cycle Assess 15:79–89

Dewaele J, Pant R, Schowanek D (2006) Comparative life cycle assessment (LCA) of Ariel “Actif à froid” (2006), a laundry detergent that allows to wash at colder wash temperatures, with previous Ariel laundry detergents (1998, 2001), http://www.scienceinthebox.com/en_UK/pdf/Ariel%20Actif%20a%20Froid%20LCA%20report%20Nov%202006.pdf. Accessed 17 Dec 2010

DID list (2007) Detergent Ingredient Database (DID list) – 2007 version. http://ec.europa.eu/environment/ecolabel/ecolabelled_products/categories/did_list_en.htm (accessed 17/12/2010)

DID list Part B (2004) Detergent ingredients database version 30 June 2004. http://ec.europa.eu/environment/ecolabel/ecolabelled_products/categories/did_list_en.htm. Accessed 17 Dec 2010

Ecolabel EU (1995) Commission decision of 25 July 1995 establishing the ecological criteria for the award of the community ecolabel to laundry detergents. Official J European Communities L217:0014–0030, 95/365/EC

Eskeland MB, Svanes E (2004) The harmonised detergent ingredient database ("DID list") for eco-labelling. Final report. Ecolabelling Norway, Service Contract B4-3040/2002/335566/MAR/D3

European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC) (2001) Aquatic toxicity of mixtures, ECETOC report No.80, Brussels (Belgium)

European Commission (2010) ESIS: European chemical substances information system. http://ecb.jrc.ec.europa.eu/esis/. Accessed 3 Dec 2010

EUSES v2.1, the European Union System for the Evaluation of Substances, version 2.1 (2008) National Institute for Public Health and the Environment (RIVM), the Netherlands, http://ecb.jrc.ec.europa.eu/euses. Accessed 17 Dec 2010

Goedkoop MJ, Heijungs R, Huijbregts M, De Schryver A, Struijs J, Van Zelm R (2008) ReCiPe 2008, a life cycle impact assessment method which comprises harmonised category indicators at the midpoint and the endpoint level; first edition report I: characterisation; 6 January 2009. http://www.lcia-recipe.net. 17 Dec 2010

Hauschild M, Wenzel H (1998) Environmental assessment of products, vol 2: scientific background. Chapman & Hall, London

Hauschild M, Huijbregts M, Jolliet O, Macleod M, Margni M, van de Meent D, Rosenbaum RK, McKone TE (2008) Building a model based on scientific consensus for life cycle impact assessment of chemicals: the search for harmony and parsimony. Environ Sci Technol 42:7032–7037

Heijungs R, Guinée JB, Huppes G, Lankreijer RM, Udo De Haes HA, Wegener Sleeswijk A, Ansems AMM, Eggels PG, Van Duin R, De Goede HP (1992) Environmental life cycle assessment of products. Guide LCA. CML Leiden, The Netherlands

Huijbregts MAJ (2010) Department of Environmental Science. Radboud University Nijmegen, The Netherlands, Personal communication. 15/10/2010

Larsen HF, Hauschild M (2007) Evaluation of ecotoxicity effect indicators for use in LCIA. Int J Life Cycle Assess 12(1):24–33

Nitschke L, Malcomber I, Tibazarwa C, Steber J (2007) Is the Ecolabel DID list a useful environmental evaluation tool for detergent-like consumer products? Tenside Surf Det 44(3):155–159

European Commission (1999) Commission decision of 10 June 1999 establishing the ecological criteria for the award of the community Eco-label to laundry detergents (1999/476/EC). Official J European Communities L 187:52–68, 20.7.1999

Pant R, Van Hoof G, Schowanek D, Feijtel TCJ, de Koning A, Hauschild MZ, Pennington DW, Olsen SI, Rosenbaum R (2004) Comparison between three different LCIA methods for aquatic ecotoxicity and a product environmental risk assessment: Insights from a detergent case study within OMNIITOX. Int J Life Cycle Assess 9(5):295–306

Pennington DW (2004) Editorial: increasing the acceptance and practicality of toxicological effects in LCA. Int J Life Cycle Assess 9(5):281

Rosenbaum R, Bachmann TM, Gold LS, Huijbregts MAJ, Jolliet O, Juraske R, Koehler A, Larsen HF, MacLeod M, Margni M, McKone TE, Payet J, Schuhmacher M, van de Meent D, Hauschild MZ (2008) USEtox—the UNEP-SETAC toxicity model: recommended ChFs for human toxicity and freshwater ecotoxicity in life cycle assessment. Int J Life Cycle Assess 13 (7):532–546

Saouter E, Van Hoof G (2002) A database for the life-cycle assessment of Procter & Gamble laundry detergents. Int J Life Cycle Assess 7(2):103–114

Saouter E, Van Hoof G, Feijtel TCJ, Owens JW (2002) The effect of compact formulations on the environmental profile of Northern European granular laundry detergents Part II: Life Cycle assessment. Int J Life Cycle Assess 7(1):27–38

U.S. National Library of Medicine (2009) Hazardous Substances Data Bank (HSDB). http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB. Accessed 3 Dec 2010

U.S. National Library of Medicine (2010) ChemIDplus Advanced. http://chem.sis.nlm.nih.gov/ChemIDplus/. Accessed 3 Dec 2010

USEPA (2009a) Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.00. United States Environmental Protection Agency, Washington, DC

USEPA (2009b) ECOSAR (Ecological Structure Activity Relationships) v. 1.00. OPPT—Risk Assessment Division

USEPA (2010) Ecotox Release 4.0. http://cfpub.epa.gov/ecotox/. Accessed 7 Jan 2011

USEtox Development Team (2010) Database for organic substances 1.01. http://redigering.sitecore.dtu.dk/Sites/usetox/howtoget/downloadmodel.aspx. Accessed 17 Dec 2010

Van Hoof G, Schowanek D, Feijtel TCJ (2003) Comparative life-cycle assessment of laundry detergent formulations in the UK: Part I. Environmental fingerprint of five detergent formulations in 2001. Tenside Surfact Det 40:266–275